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Model Ion Abundances for Comet Halley

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Abstract

Our computer model for comet comae has been applied to predict ion abundances for comet Halley. We assume that the volatile component of the nucleus is 85% water and that the remaining volatile molecules are composed of carbon, nitrogen, oxygen, and sulfur. Model parameters such as heliocentric distance, size, and albedo are chosen to be consistent with the 13-14 March 1986 encounter of the Giotto spacecraft with the comet. Photoprocesses, gas-phase chemical kinetics, coma energy balance including a separate electron temperature, multifluid hydrodynamics with a transition to free molecular flow, fast streaming atomic and molecular hydrogen, and counter and cross streaming of species in the coma-solar wind interaction are taken into consideration. A comparison of the model results is made with preliminary data from the ion mass spectrometer at 6000 and 1500 km from the nucleus. We find good overall agreement. The implication of the coma physics and chemistry are discussed.

Key words: Ion Mass Spectrometer Data, Coma Model

This is a progress report on the application of our coma model with solar wind interaction to the ion abundances as measured by Balsiger et al. (1986) with the ion mass spectrometer (IMS) on the Giotto spacecraft. We emphasize the preliminary nature of this report; several improvements on our model are incomplete. Part of the discussion, which includes the sulfur chemistry, is based on molecular production rates that are more appropriate for Comet Halley during the fly-by of Giotto, while the solar wind interaction part that is needed for the description of the ion species outside of the contact surface is based on earlier production rates that are more appropriate for the Vega fly-bys and uses a solar wind density that is too high by a factor of two.

For the newer calculations, we assume a heliocentric distance of $r=0.89\text{au}$, an albedo of $A=0.03$, an infrared emissivity of $E=0.97$, and a radius of $R=3\text{km}$ equivalent to the active area of the nucleus with hemispherical illumination. With these assumptions the production rate is $Q=5.1 \times 10^{29}$ molecules s^{-1} . For comparison,

Krankowsky et al. (1986) report a total gas production rate of $6.9 \times 10^{28} \text{ s}^{-1}$. The coma gas produced on the sunlit hemisphere spreads over the nucleus and the neutral component expands iniformlly, while the ion component expands uniformly only until it interacts with the solar wind.

We assume the composition of the nucleus as given in Table I.

Table I

| <u>Assumed Composition of the Nucleus</u> | | |
|---|-------|---------------------|
| H_2O | 85.0% | identified |
| H_2CO | 3.5 | identified |
| CO_2 | 3.0 | identified |
| CH_4 | 2.5 | |
| CO | 2.0 | possibly identified |
| N_2 | 1.2 | |
| CS_2 | 1.0 | |
| H_2CO_2 | -1.0 | |
| HCN | | possibly identified |
| CH_3CN | | |
| NH_2CH_3 | | |
| $\text{H}_2\text{C}_3\text{H}_2$ | 0.8 | |
| NH_3 | | |
| C_2H_2 | | |

It is our goal to vary the composition for the nucleus using neutral molecules that have been identified in Comet Halley, but supplemented with other molecules, until our model predicts ion abundances that are in reasonable agreement with the measurements from the IMS. Among the identified molecules are H_2O , with an abundance of ~80% (Krankowsky et al., 1986), CO_2 with an abundance of 1.5% (Combes et al., 1986) to 3.5% (Krankowsky et al., 1986) relative to H_2O , HCN (Bookalee-Morvan et al., 1986) at the <1% level, at possibly H_2CO and CO (Combes et al., 1986).

Our model consists of two sections: (1) the radially symmetric inner coma and (2) the axi-symmetric solar wind interaction. The radially symmetric inner coma part models photoprocesses with wavelength-dependent attenuation, gas-phase chemical kinetics for H-, C-, N-, O-, and S- compounds, coma energy balance including a separate determination of the electron temperature which enhances electron-collisional dissociation and ionization, and multifluid hydrodynamics for fast streaming atomic and molecular hydrogen and a transition to free molecular flow. The radially symmetric part of the model is also extended into the axi-symmetric part for the neutral coma molecules. The axi-symmetric solar wind interaction models the photo-processes and the chemical kinetics consistently with the above radially symmetric part. It also allows for counter and cross streaming of neutrals and ions.

mass loading of the solar wind and the bow shock and the contact surface, but magnetic fields are not included. The model has been described in greater detail by Huebner et al. (1986).

According to our model the solar wind has two main effects on the ion densities when compared to model calculations without solar wind interaction: (1) It enhances the ion densities outside of the contact surface by about a factor of two, simulating a pile-up of ions and (2) it steepens the density profiles outside of this enhanced region. Since our assumed gas production rate for the comet and the solar wind density were both too high by about a factor of two when compared to values more appropriate during the Giotto encounter with Comet Halley, our model predicts the contact surface at too large a distance from the nucleus. Reducing the production rate and the solar wind density will bring the contact surface closer to the observed position, but we cannot predict in which direction the ion density enhancement will go. However, our model results are in qualitative agreement with the measured count rates obtained with the high-intensity spectrometer (HIS) sensor of the IMS (Balsiger et al., 1986). The sharp decay in our model of H_3O^+ with increasing distance, followed by less steep decays of H_2O^+ , OH^+ , and finally O^+ , are also in agreement with the behavior observed in the results from the IMS.

Inside as well as outside of the contact surface, our model reproduces the gross features of the three mass/charge (M/Q) groups in the spectrum obtained with the IMS. However, significant adjustments will have to be made to the assumed initial composition (Table I) and to the chemical reaction network in our model before the details in the M/Q spectrum can be compared with the IMS results. In particular, the sulfur chemistry has been added to our model only recently and may be incomplete. The NH_4^+ abundance will have to be increased to enhance NH_4^+ production which has the same M/Q value as H_2O^+ , to bring the relative abundance of M/Q=18 to M/Q=19 into better agreement. At present, isotopes are completely ignored in our model. Table II summarizes the current status of ions in our model for the M/Q values from 12 to 55. In conjunction with this, it is of interest to comment on the presentation by Krankowsky on sulfur chemistry earlier in these proceedings: For M/Q=45, our current model gives a larger contribution from HCS^+ than from HCO_2^+ .

Table II

Dominant ions in M/Q bins (isotopes are ignored)

| | | | |
|----|------------------------------------|----|----------------------------|
| 12 | C^+ | 34 | H_2S^+ |
| 13 | CH^+ | 35 | H_3S^+ |
| 14 | CH_2^+, N^+ | 36 | C_3^+ |
| 15 | CH_3^+, NH^+ | 37 | C_3H^+, H_3O^+, H_2O |
| 16 | CH_4^+, O^+, NH_2^+ | 38 | $C_2N^+, C_3H_2^+$ |
| 17 | OH^+, NH_3^+, CH_5^+ | 39 | $C_3H_3^+$ |
| 18 | H_2O^+, NH_4^+ | 40 | $C_3H_4^+, CH_2CN^+$ |
| 19 | H_3O^+ | 41 | $C_3H_5^+$ |
| 20 | | 42 | |
| 21 | | 43 | CH_3CO^+ |
| 22 | | 44 | $CO_2^+, CS^+, C_3H_8^+$ |
| 23 | | 45 | HCS^+, HCO_2^+ |
| 24 | C_2^+ | 46 | $H_2CO_2^+, NS^+, H_2CS^+$ |
| 25 | C_2H^+ | 47 | HNS^+, H_3CS^+ |
| 26 | $C_2H_2^+$ | 48 | SO^+ |
| 27 | $C_2H_3^+, HCN^+$ | 49 | HSO^+ |
| 28 | $H_2CN^+, CO^+, N_2^+, C_2H_4^+$ | 50 | $C_4H_2^+$ |
| 29 | $HCO^+, C_2H_5^+, N_2H^+$ | 51 | $C_4H_3^+$ |
| 30 | $H_2CO^+, C_2H_6^+, NO^+, CH_4N^+$ | 52 | $C_3H_2N^+$ |
| 31 | CH_2OH^+, HNO^+ | 53 | $C_4H_5^+$ |
| 32 | S^+, O_2^+ | 54 | |
| 33 | HS^+, O_2H^+ | 55 | $C_3H_3O^+, C_4H_7^+$ |

Balsiger, H., K. Altwegg, F. Buhler, J. Geiss, A. G. Ghielmetti,
 B. E. Goldstein, R. Goldstein, W. T. Huntress, W. -H. Ip,
 A. J. Lazarus, A. Meier, M. Neugebauer, U. Rettemund,
 H. Rosenbauer, R. Schwenn, R. D. Sharp, E. G. Shelley,
 E. Ungstrup, and D. T. Young, *Nature* 321, 330 (1986).

Combes, M., V. Moroz, J. F. Crifo, J. P. Bibring, N. Coron,
 J. Crovisier, T. Encrenaz, N. Sanko, A. Grigoriev,
 D. Bockelee-Morvan, R. Gispert, C. Emerich, J. M. Lamarre
 F. Rocard, V. Krasnopolsky, and T. Owen, this report (1986).

Krankowsky, D., P. Lammerzah, I. Herrwerth, J. Woweries,
 P. Eberhardt, U. Dolder, U. Herrmann, W. Schulte,
 J. J. Barthelier, J. M. Illiano, R. R. Hodges, and
 J. H. Hoffman, *Nature* 321, 326 (1986).

Bockelee-Morvan, D., J. Crovisier, D. Despois, T. Forveille,
 E. Gerard, J. Schrami, and C. Thum, this report (1986).

Huebner, W. F., D. C. Boice, J. J. Keady, H. U. Schmidt, and
 R. Wegmann, *IAU Colloquium*, in press (1986).